

## Supporting Information

### **An efficient cluster model to describe oxygen reduction reaction activity of metal catalysts: A combined theoretical and experimental study**

Liting Cui<sup>a</sup>, Haining Wang<sup>\*a</sup>, Sian Chen<sup>a</sup>, Jin Zhang<sup>a</sup>, Yan Xiang<sup>a</sup> and Shanfu Lu<sup>\*a</sup>

<sup>a</sup> Beijing Key Laboratory of Bio-inspired Energy Materials and Devices, School of Space and Environment, Beihang University, Beijing, 100191, China.

Emails: hwang@buaa.edu.cn, lusf@buaa.edu.cn.

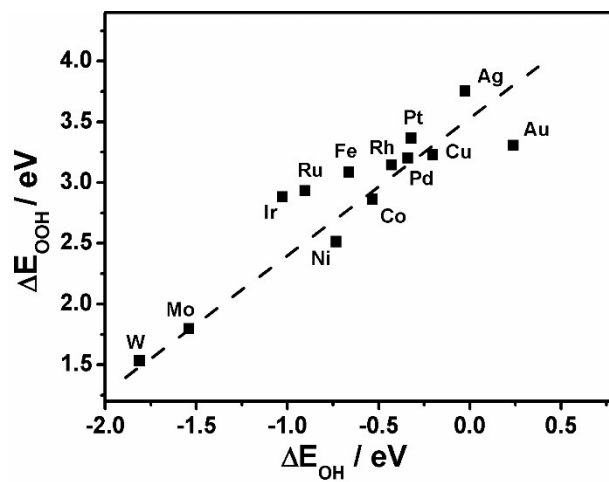


Fig. S1 The scaling relation between binding energies of OH and OOH.

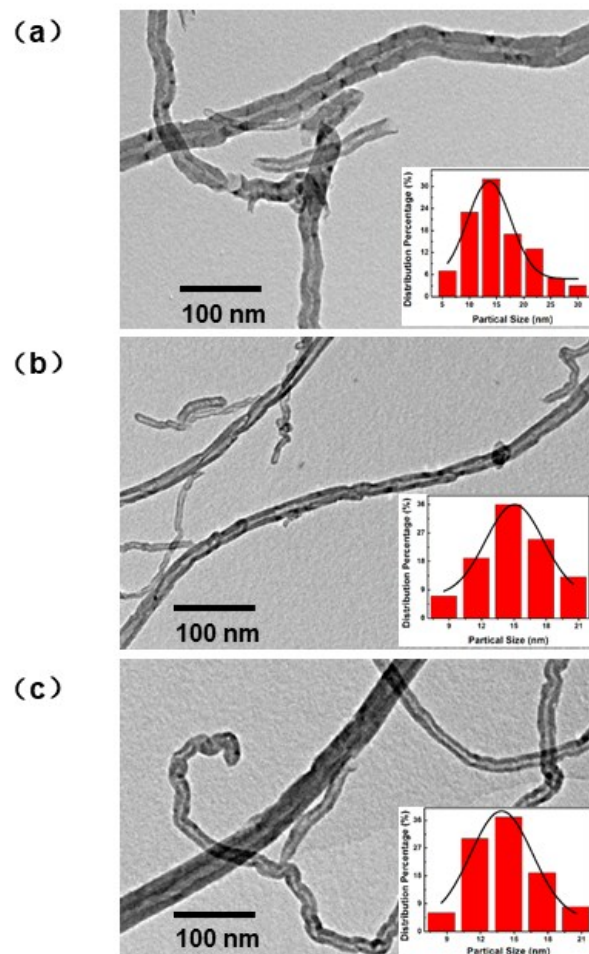


Fig. S2 TEM images of (a) Ag/CNTs, (b) Ag/OH-CNTs and (c) Ag/COOH-CNTs respectively.

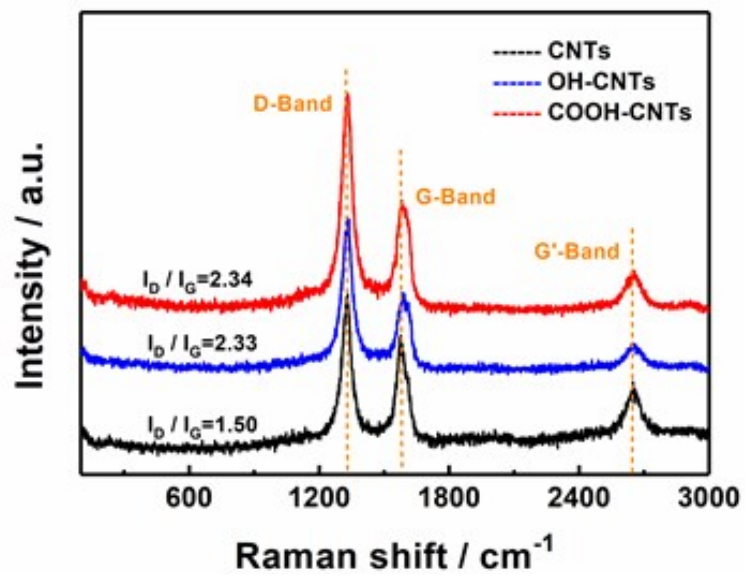


Fig. S3 The Raman spectra of the CNT, OH-CNTs and COOH-CNTs respectively.

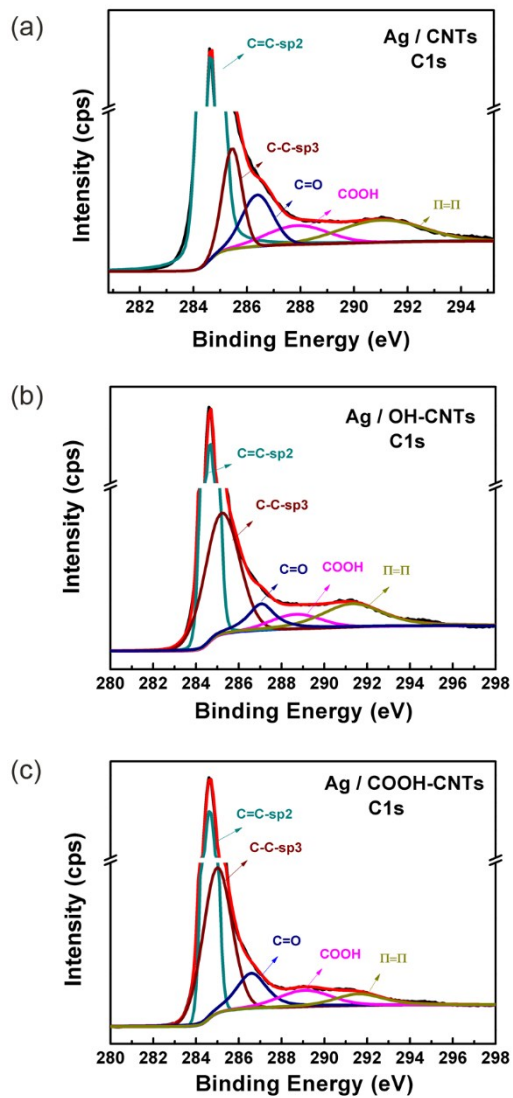


Fig. S4 C1s XPS spectra of (a) Ag/CNT, (b) Ag/OH-CNTs and (c) Ag/COOH-CNTs respectively.

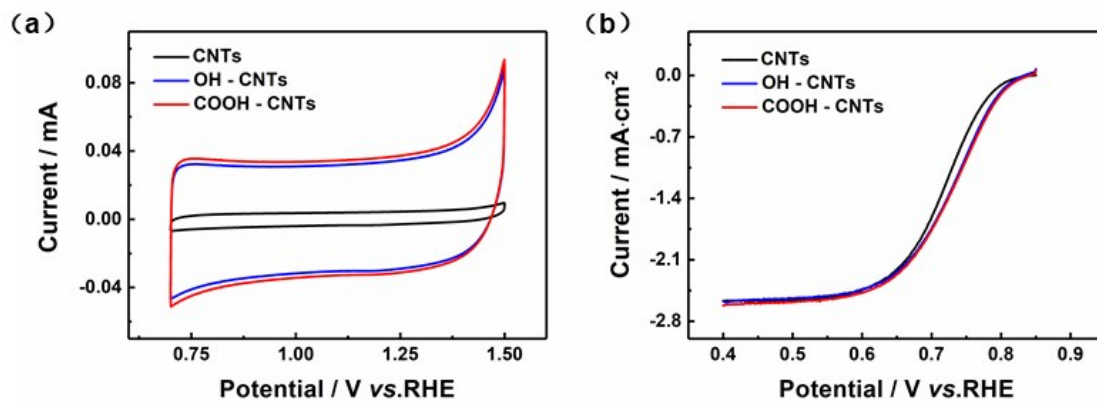


Fig. S5 (a) CV curves of CNTs, OH-CNTs and COOH-CNTs in nitrogen saturated 0.1 M KOH solution at a scan rate of 50 mV s<sup>-1</sup>. (b) LSV curves of different CNTs in oxygen saturated 0.1 M KOH solution at a scan rate of 10 mV s<sup>-1</sup> with electrode rotation rate of 1600 rpm.

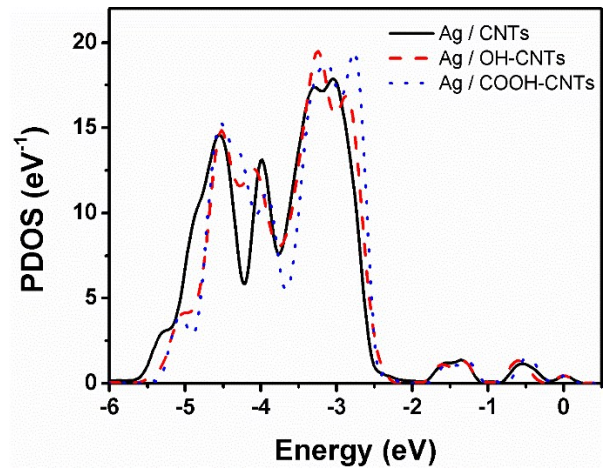


Fig. S6 PDOS curves of Ag supported on different CNTs.